

Control of Rydberg atoms to perform Grover's search algorithm

C. RANGAN, J. AHN, D. N. HUTCHINSON and P. H. BUCKSBAUM

FOCUS Center, Physics Department, University of Michigan, Ann Arbor, MI 48109 -1120, USA

(Received 15 February 2002; revision received 27 May 2002)

Abstract. It is shown that Grover's search algorithm can be implemented on a Rydberg atom data register using a short terahertz half-cycle pulse. Using optimal control theory, a shaped terahertz pulse is designed that can perform the search algorithm better than an unshaped half-cycle pulse. Starting from an initial wave packet, it is shown that it is possible to use the search algorithm to synthesize single-energy eigenstates.

1. Introduction

In this paper, we show that Grover's search algorithm [1] can be performed on a Rydberg atom data register using a broadband, terahertz half-cycle pulse (HCP). The search algorithm is a quantum mechanical method of searching an N -state database to find a single bit of information stored in one of the states. A general understanding of the search algorithm can be obtained from reference [2]. The database consists of quantum states that are otherwise indistinguishable except for the relative phase differences between them. The algorithm transforms this phase information into amplitude information, which can then be measured easily. The algorithm has been implemented in several physical systems [3–9]; here we present an implementation in a Rydberg atom.

We present three related, but different, results. Using an impulse model of the HCP, it is shown that the phase retrieval performed by the HCP is closely related to the inversion-about-the-average operation central to the search algorithm. Using optimal control theory, shaped terahertz pulses are designed that can perform the search algorithm better than unshaped HCPs. Finally, it is shown that a broadband terahertz pulse can be used to drive a Rydberg wave packet population into a single eigenstate.

The motivation for this research is the implementation of Grover's search algorithm [1] in a Rydberg atom. Figure 1 shows a schematic of this process. In our implementation of the quantum search algorithm, the data register is a Rydberg wave packet, i.e. a superposition of several eigenstates. In the experimental system, the $24p$ through $29p$ states of Cesium are used. Each eigenstate acts as a bit, and the information is stored in the phases of these eigenstates. A binary encoding is used: if the phase of an eigenstate relative to a reference state is 0, then the bit value is binary 0; if the phase of an eigenstate is π relative to a reference,

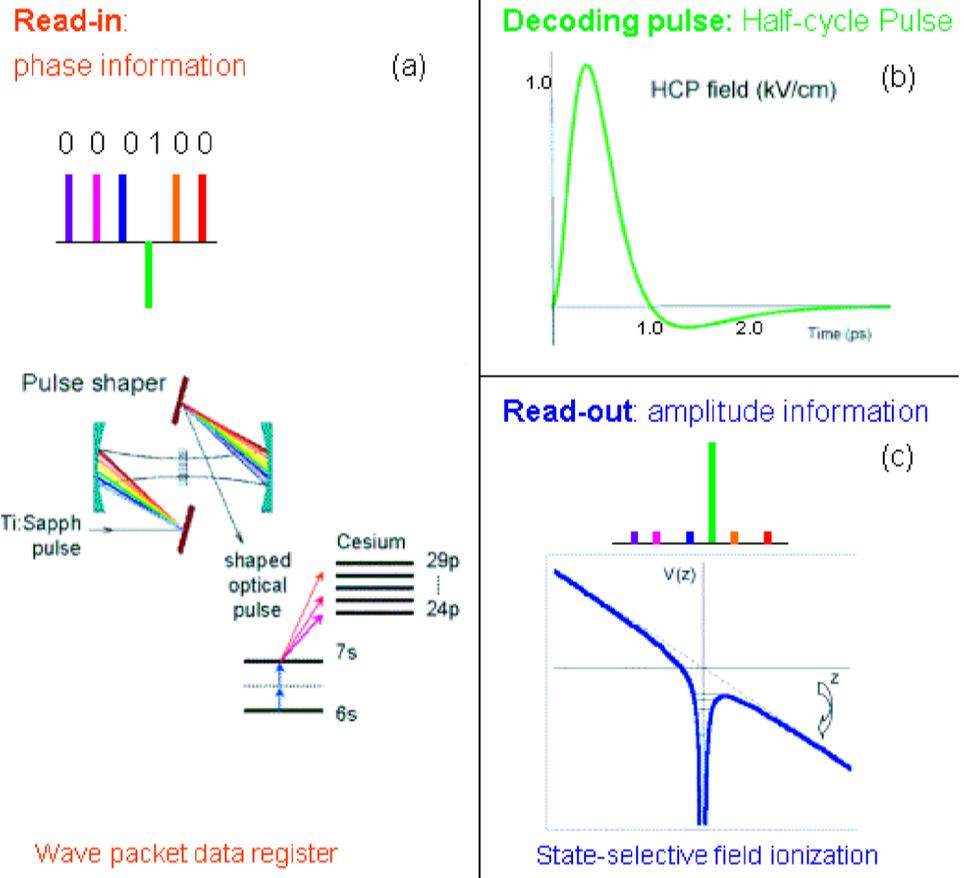


Figure 1. Schematic of the phase retrieval process in a Rydberg atom. (a) Read-in of data by excitation of a Rydberg wave packet. (b) Electric field of the terahertz half-cycle pulse that performs the search algorithm. (c) Measurement of decoded information by state-selective field ionization.

then the bit value is binary 1. The search space is restricted to those wave packets one of whose constituent orbitals has its phase reversed. Thus an initial wave packet with the constituent orbitals $|24p\rangle$ to $|29p\rangle$ of Cesium, with the phase of the $|26p\rangle$ orbital reversed with respect to the others is represented by the column vector $(1, 1, -1, 1, 1, 1)^T / \sqrt{N}$, where $N = 6$. The data register is loaded by exciting the Rydberg atom using a shaped, optical pulse [10]. A schematic of this process is shown in figure 1(a).

This phase information is converted to amplitude information by a terahertz, broadband, half-cycle pulse (HCP) [11], shown in figure 1(b). The half-cycle pulse reveals the marked bit by redistributing the Rydberg population so that a significant fraction of the electron's probability density lies in the orbital that was initially 180° out of phase with respect to the other orbitals. This amplitude information is read out by state-selective field ionization of the Rydberg atoms. This is a well-established experimental method—the field ionization signal provides a temporal map of the electronic probability distribution, indicated

schematically in figure 1(c). Thus the half-cycle pulse performs the search by converting the phase information (which state has its phase reversed) into amplitude information (which state has the largest amplitude), which can then be measured.

2. Phase retrieval and the Grover's search algorithm

The initial experiment and calculations presented in reference [11] show that the terahertz pulse amplifies the phase-flipped orbital of a Rydberg wave packet data register. Calculations using both an impulse model and a fitted model of the HCP (full solution to the time-dependent Schrödinger equation) agree very well with the experimental results. This indicates that the impulse approximation, when the width of such a half-cycle pulse is much shorter than the Kepler orbital period of the wave packet, is valid for this system. Therefore, we use the impulse model to understand the how the HCP performs the database search.

The action of the half-cycle pulse on the initial wave packet can be written (in atomic units) as

$$|\Psi(T)\rangle = \exp\left(-i \int_0^T E(t)dt\right)|\Psi(0)\rangle \quad (1)$$

In the impulse limit, when the pulse width is much smaller than the Kepler orbital period, the electron does not evolve while the pulse is on. The pulse transfers a momentum Q to the electron, equal to the integrated area of the electric field as a function of time:

$$|\Psi(T)\rangle = \exp(iQz)|\Psi(0)\rangle \quad (2)$$

The matrix elements of the impulse operator in the energy basis can be written as

$$M_{n'l'nl} = \langle n', l', m = 0 | \exp(iQz) | n, l, m = 0 \rangle \quad (3)$$

For the database states ($24p$ to $29p$ of Cs),

$$M_{n'l'nl} = \langle n'p | \exp(iQz) | np \rangle \quad (4)$$

As this operator connects states of the same parity, only the even powers of Qz contribute to the matrix elements, and the matrix elements are all real. This is not a requirement for the search algorithm, but an extra symmetry imposed by the experimental implementation. These matrix elements can be calculated analytically [11]. Examining the matrix elements as a function of Q , the total momentum transferred by the HCP [12], we see that the diagonal matrix elements (that connect a database state to itself) and the off-diagonal matrix elements (that connect a database state to its neighbors in the database) both oscillate as a function of Q . For a range of Q -values around Q_0 , the diagonal elements of the M -matrix have the opposite sign from the off-diagonal elements. At $Q = Q_0$, the magnitudes of the off-diagonal elements are roughly equal, so we can write the action of the matrix on the initial state as

$$\begin{pmatrix} -a & b & b & b & b & b \\ b & -a & b & b & b & b \\ b & b & -a & b & b & b \\ b & b & b & -a & b & b \\ b & b & b & b & -a & b \\ b & b & b & b & b & -a \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ -1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{N}} = \begin{pmatrix} -a + (N - 3)b \\ -a + (N - 3)b \\ +a + (N - 1)b \\ -a + (N - 3)b \\ -a + (N - 3)b \\ -a + (N - 3)b \end{pmatrix} \frac{1}{\sqrt{N}} \quad (5)$$

If one of the states is marked, i.e. has its phase reversed with respect to those of the others, the multimode interference conditions are appropriate for constructive interference to the marked state, and destructive interference to the others. That is, the population in the marked bit is amplified. The form of this matrix is identical to that obtained through the inversion about the average procedure in Grover’s search algorithm. This operator produces a contrast in the probability density of the final states of the database of $(a + (N - 1)b)^2/N$ for the marked bit versus $(a - (N - 3)b)^2/N$ for the unmarked bits; where, N is the number of bits in the data register.

3. Optimal phase retrieval via shaped terahertz pulses

In the physical system, phase retrieval is not performed with the efficiency expected from the matrix M in equation (5). A major reason for this is that the far off-diagonal matrix elements are, in general, smaller than the near off-diagonal elements. The amplification of population in the marked bit occurs by ‘diffusion’ (to borrow Grover’s term) of population from the nearby bits with a relative phase between them. Since the overlap between states that are far apart in the register is small, the far off-diagonal terms in the matrix are also small. If the marked bit is one of the outer states in the register, its phase retrieval is not as efficient as expected from the matrix.

This effect was seen in the published experiment [11] where the $26p$ and $27p$ states were retrieved with higher fidelity than the $25p$ and $28p$ states. This problem has been addressed in a recent theoretical work [13], where, by using a shaped terahertz pulse designed by optimal control theory, it is shown that the phase retrieval can be performed successfully for all but the two outermost database orbitals. The challenge here is to design a pulse that does more than perform a unitary transformation; it should perform an algorithm. That is, the same terahertz pulse should optimally take several initial eigenstates to the appropriate final state. Explicitly,

$$\begin{aligned} (1 \quad -1 \quad 1 \quad 1 \quad 1 \quad 1)^T &\rightarrow (0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0) \\ (1 \quad 1 \quad -1 \quad 1 \quad 1 \quad 1)^T &\rightarrow (0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0) \\ (1 \quad 1 \quad 1 \quad -1 \quad 1 \quad 1)^T &\rightarrow (0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0) \\ (1 \quad 1 \quad 1 \quad 1 \quad -1 \quad 1)^T &\rightarrow (0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0) \end{aligned} \quad (6)$$

We use the standard formalism of optimal control theory [14–16], where the optimal field $E(t)$, $0 \leq t \leq T$ is calculated by optimizing an unconstrained functional

$$\bar{J} = \langle \Psi(T) | P_k | \Psi(T) \rangle - \int_0^T dt l(t) |E(t)|^2 - 2\Re \langle \dot{\lambda}(t) | \Psi(t) \rangle - \int_0^T dt 2\Re \langle \lambda(t) | iH | \Psi(t) \rangle \quad (7)$$

Here, P_k is the operator that must be optimized at time T (the flipped bit population). The parameter $l(t)$ imposes a cost on the total energy of the pulse, and makes the field go smoothly to zero at the temporal end points. The third and fourth terms are the constraints imposed by the Schrödinger equation. To find the electric field that simultaneously optimizes several unitary operations (i.e. start from several initial states, and go to the appropriate final states), we redefine the optimal control problem. We consider an initial state that is a product state of independent wave packets with singly flipped orbitals.

$$|\Psi(0)\rangle = |\Psi_{25p}^1\rangle \otimes |\Psi_{26p}^2\rangle \otimes |\Psi_{27p}^3\rangle \otimes |\Psi_{28p}^4\rangle \quad (8)$$

where $|\Psi_{26p}\rangle = (1 \quad 1 \quad -1 \quad 1 \quad 1 \quad 1)^T \frac{1}{\sqrt{N}}$

The terahertz pulse acts simultaneously, but independently on all these wave packets. The desired final state is also a product state of independent wave packets with the flipped bit correctly decoded.

$$|\Psi(T)\rangle = |25p\rangle \otimes |26p\rangle \otimes |27p\rangle \otimes |28p\rangle \quad (9)$$

At every time step, the updated THz field is found by using a modified version of the algorithm used to optimize a single target state [13]. Using this new method, we find the terahertz pulse that detects any flipped orbital of the N -bit data register.

We have chosen a fixed pulse length T of roughly 8ps. The THz field that optimizes the population in any marked state is shown in figure 2(a). The pulse has a strong initial lobe similar to the positive lobe of a half-cycle pulse. This pulse clearly retrieves the marked bit information much better than an unshaped HCP. The evolution of the wave packet as a function of time while the optimal pulse is on, seen in figure 2(b) and figure 2(c) shows that the HCP-like lobe does the phase retrieval, and the rest of the pulse performs the amplification of the population in the marked bit. This corresponds well with our impulse-model understanding of the search algorithm.

The optimal shaped terahertz pulse has some interesting characteristics. Notably, the strong peaks in the spectrum and the Husimi distribution (seen in figure 3(a) and figure 3(b) respectively) do not correspond to resonances between the energy levels of the selected state basis. The optimal terahertz pulse does not drive the system to any particular resonant condition. Instead, it alters the phases of the constituent orbitals of the wave packet so that they interfere to produce the desired probability distribution. Another interesting feature of this optimal pulse is that the peak field of roughly 1 kV cm^{-1} lasts for roughly 0.5ps. For a wave packet centred at $n = 26$, this field, which is beyond the field ionization limit, lasts for more than half the Kepler period ($\sim 2\pi n^3$). Yet, 99% of the population remains in

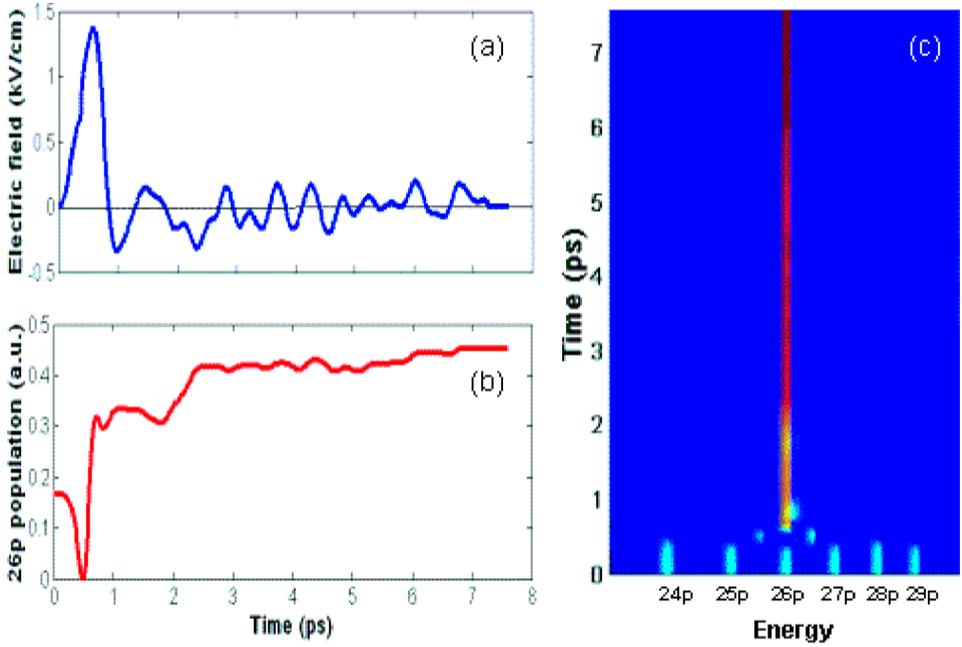


Figure 2. Shaped terahertz pulse that optimally performs the phase retrieval. (a) Electric field of the pulse as a function of time. (b) Target state population during the pulse as a function of time. (c) Temporal evolution of the Rydberg wave packet during the shaped terahertz pulse.

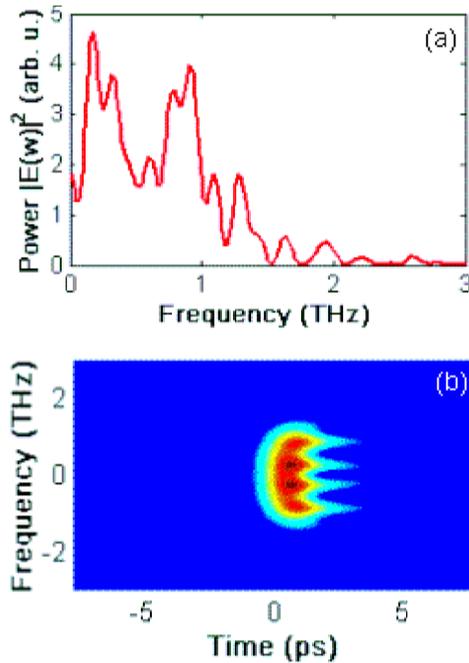


Figure 3. (a) Fourier transform and (b) Husimi distribution of the shaped terahertz pulse.

the selected state basis. This feature is an example of interferometric stabilization [17], seen in other atomic systems.

4. Creating states outside the database

According to Grover, 'The quantum search algorithm can be looked at as a technique for synthesizing a particular kind of superposition—one whose amplitude is concentrated in a single basis state' [18]. This is exactly what is done in the general algorithm. The question is: Can we use the HCP to drive amplitude into eigenstates other than those within the database? These outside states are initially unpopulated. For example, if the initial wave packet has population in the 24*p* to 29*p* 'database' states, we would like to use the HCP to produce a 27*s*-eigenstate. In the Cesium spectrum, the *s*-states are spectrally separated from the database states. The graph of the matrix elements between the database states and the target state as a function of *Q* in figure 4(a) shows that in order to produce an *s*-state, all the

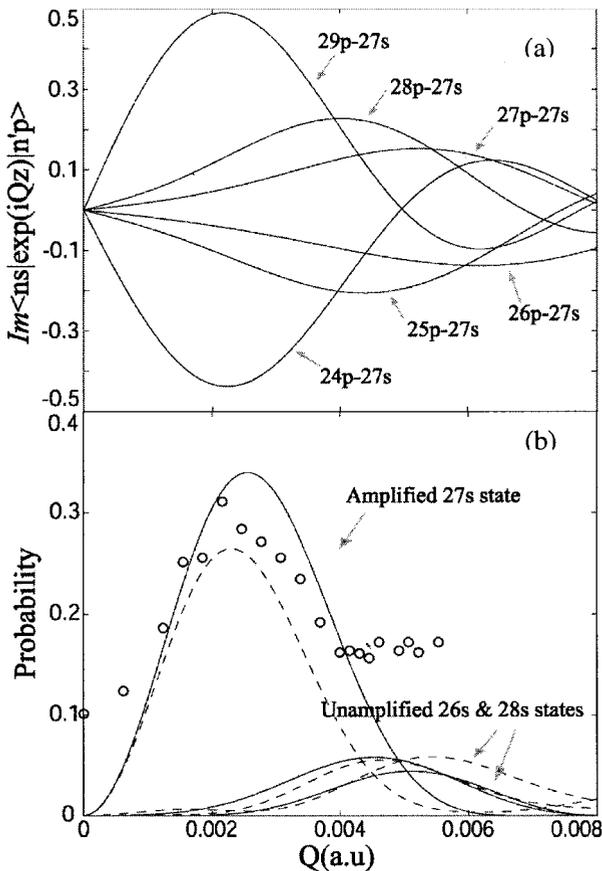


Figure 4. (a) Matrix elements of the HCP interaction between the database states and the desired non-database states as a function of the impulse Q . (b) Experimental (circles) and calculated (lines) results of the desired non-database state population as a function of Q . The solid line corresponds to the impulse model calculation, and the dashed line corresponds to a full calculation by solving the time-dependent Schrödinger equation.

higher p -states have to be in phase, but out of phase with the all the lower p -states [12]. An impulse interacting with a wave packet that has this phase structure creates the constructive interference condition for that s -state. The phase structure of the initial wave packet that produces the $|27s\rangle$ state (that is in between the $|26p\rangle$ and $|27p\rangle$ states) is $(1, 1, 1, -1, -1, -1)/\sqrt{N}$. The experimental spectra of the decoded wave packet as a function of the peak field of the HCP show that s -states appear at a HCP strength of $Q = 0.0024$ a.u. as seen in figure 4(b). Previous experiments have shown that an HCP can interact with a Rydberg eigenstate to produce a wave packet [19]. This experiment shows that the inverse is also achievable—a properly programmed wave packet can be driven towards an eigenstate by a broadband HCP interaction.

5. Scaling

The advantage of this method is that the search is completed by a single query (a single HCP) by exploiting the massive parallelism obtained by having many identical Rydberg atoms for the measurement. The extension of the Rydberg atom implementation of the search algorithm to larger registers is limited. The scaling of the peak HCP with change in n , the principal quantum number of the marked bit, is suggested by the form of the impulse operator $\exp(iQz)$. The average radial extent of a Rydberg state scales as n^2 . For marked bits with different n -values, the Q of the HCP that retrieves them can be expected to scale as n^{-2} [12]. Experimentally, it is possible to load a larger register at a higher central n -value, but the field-ionization signal loses resolution in that regime. This limits the size of the Rydberg register. The Rydberg system has limited scaling capability, but otherwise contains all of the features needed to execute the algorithm [20].

6. Conclusions

We have shown that Grover's search algorithm can be performed optimally on a Rydberg atom data register. Optimal control theory can be extended to design broadband terahertz pulses for the control of an atom to execute an algorithm. A half-cycle pulse can be used to drive a wave packet towards a single energy eigenstate. These results provide the motivation for terahertz pulse shaping and control.

References

- [1] GROVER, L. K., 1997, *Phys. Rev. Lett.*, **79**, 325.
- [2] GROVER, L. K., 1998, *Science*, **280**, 228.
- [3] CHUANG, I. L., GERSHENFELD, N., and KUBINEC, M., 1998, *Phys. Rev. Lett.*, **80**, 3408.
- [4] BIHAM, E., BIHAM, BIRON, D., *et al.*, 1999, *Phys. Rev. A*, **60**, 2742.
- [5] HOWELL, J. C., and YEAZELL, J. A., 2000, *Phys. Rev. Lett.*, **85**, 198.
- [6] KWIAT, P. G., MITCHELL, J. R., SCHWINDT, P. D. D. *et al.*, 200, *J. Mode. Opt.*, **47**, 257.
- [7] KWEK, L. C., OH, C. H., SINGH, K., *et al.*, 2000, *Phys. Rev. A*, **267**, 24.
- [8] MANG, F., 2001, *Phys. Rev. A*, **63**, 052308.
- [9] SCULLY, M. O., and ZUBAIRY, M. S., 2001, *P. Natl. Acad. Sci. (USA)*, **98**, 9490.
- [10] AHN, J., WEINACHT, T. C., and BUCKSBAUM, P. H., 2000, *Science*, **287**, 463.
- [11] AHN, J., HUTCHINSON, D. N., RANGAN, C., and BUCKSBAUM, P. H., 2001, *Phys. Rev. Lett.*, **86**, 1179.

- [12] AHN, J., RANGAN, C., HUTCHINSON, D. N., and BUCKSBAUM, P. H., 2002, *Phys. Rev. A*, **66**, 22312.
- [13] RANGAN, C., and BUCKSBAUM, P. H., 2001, *Phys. Rev. A*, **64**, 33417.
- [14] PIERCE, A. P., DAHLEH, M. A., and RABITZ, H., 1988, *Phys. Rev. A*, **37**, 4950.
- [15] SHI, S., and RABITZ, H., 1990, *J. Chem. Phys.*, **92**, 364.
- [16] KOSLOFF, R., RICE, S. A., GASPARD, P., TERSIGNI, S., and TANNOR, D. J., 1989, *Chem. Phys.*, **139**, 201.
- [17] FEDOROV, M. V., and MOVESIAN, A. M., 1988, *J. Phys. B*, **21**, L155.
- [18] GROVER, L. K., 2000, *Phys. Rev. Lett.*, **85**, 1334.
- [19] TIELKING, N. E., and JONES, R. R., 1995, *Phys. Rev. A*, **52**, 1371.
- [20] MEYER, D. A., 2000, *Phys. Rev. Lett.*, **85**, 2014.